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T-Q relation and exact solution for the XYZ chain with general nondiagonal boundary terms

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Abstract

We propose that the Baxter's Q-operator for the quantum XYZ spin chain with open boundary conditions is given by the $j \to \infty$ limit of the corresponding transfer matrix with spin-j (i.e., $(2j+1)$-dimensional) auxiliary space. The associated T-Q relation is derived from the fusion hierarchy of the model. We use this relation to determine the Bethe Ansatz solution of the eigenvalues of the fundamental transfer matrix. The solution yields the complete spectrum of the Hamiltonian.

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1 Introduction

In this paper we are interested in the exact solution of the quantum XYZ quantum spin chain with most general nondiagonal boundary terms, defined by the Hamiltonian

$$H = \sum_{j=1}^{N-1} \left(J_x \sigma_j^x \sigma_{j+1}^x + J_y \sigma_j^y \sigma_{j+1}^y + J_z \sigma_j^z \sigma_{j+1}^z \right) + h_x^{(-)} \sigma_1^x + h_y^{(-)} \sigma_1^y + h_z^{(-)} \sigma_1^z + h_x^{(+)} \sigma_N^x + h_y^{(+)} \sigma_N^y + h_z^{(+)} \sigma_N^z, \tag{1.1}$$

where σ^x, σ^y, σ^z are the usual Pauli matrices, N is the number of spins, the bulk coupling constants J_x, J_y, J_z are related to the crossing parameter η and modulus parameter τ by the following relations,

$$J_x = \frac{e^{i\pi\eta}\sigma(\eta + \frac{\tau}{2})}{\sigma(\frac{\tau}{2})}, \quad J_y = \frac{e^{i\pi\eta}\sigma(\eta + \frac{1}{2} + \frac{\tau}{2})}{\sigma(\frac{1}{2} + \frac{\tau}{2})}, \quad J_z = \frac{\sigma(\eta + \frac{1}{2})}{\sigma(\frac{1}{2})},$$

and the components of boundary magnetic fields associated with the left and right boundaries are given by

$$\begin{aligned} h_x^{(\mp)} &= \pm e^{-i\pi(\sum_{l=1}^3 \alpha_l^{(\mp)} - \frac{\tau}{2})} \frac{\sigma(\eta)}{\sigma(\frac{\tau}{2})} \prod_{l=1}^3 \frac{\sigma(\alpha_l^{(\mp)} - \frac{\tau}{2})}{\sigma(\alpha_l^{(\mp)})}, \quad h_z^{(\mp)} = \pm \frac{\sigma(\eta)}{\sigma(\frac{1}{2})} \prod_{l=1}^3 \frac{\sigma(\alpha_l^{(\mp)} - \frac{1}{2})}{\sigma(\alpha_l^{(\mp)})}, \\ h_y^{(\mp)} &= \pm e^{-i\pi(\sum_{l=1}^3 \alpha_l^{(\mp)} - \frac{1}{2} - \frac{\tau}{2})} \frac{\sigma(\eta)}{\sigma(\frac{1}{2} + \frac{\tau}{2})} \prod_{l=1}^3 \frac{\sigma(\alpha_l^{(\mp)} - \frac{1}{2} - \frac{\tau}{2})}{\sigma(\alpha_l^{(\mp)})}. \end{aligned} \tag{1.2}$$

Here $\sigma(u)$ is the σ-function defined in the next section and $\{\alpha_l^{(\mp)}\}$ are free boundary parameters which specify the boundary coupling (equivalently, the boundary magnetic fields).

In solving the closed XYZ chain (with periodic boundary condition), Baxter constructed a Q-operator [1], which has now been proved to be a fundamental object in the theory of exactly solvable models [2]. However, Baxter's original construction of the Q-operator was ad hoc and its connection with the quantum inverse scattering method was not clear. It was later argued [3] that the Q-operator for the XXZ spin chain with periodic boundary condition may be constructed from the $U_q(\widehat{sl_2})$ universal L-operator whose associated auxiliary space is taken as an infinite dimensional q-oscillator representation of $U_q(\widehat{sl_2})$. (See also [4] for recent discussions on the direct construction of the Q-operator of the closed chain.) In [5], a natural set-up to define the Baxter's Q-operator within the quantum inverse scattering method was proposed for the open XXZ chain. However, the generalization of the construction to *off-critical* elliptic solvable models [6] (including the XYZ chain) is still lacking even for the closed chains.

In this paper, we generalize the construction in [5] to Baxter's eight-vertex model and propose that the Q-operator $\bar{Q}(u)$ for the XYZ quantum spin chain (closed or open) is given by the $j \to \infty$ limit of the corresponding transfer matrix $t^{(j)}(u)$ with spin-j (i.e., $(2j+1)$-dimensional) auxiliary space,

$$\bar{Q}(u) = \lim_{j\to\infty} t^{(j)}(u - 2j\eta). \tag{1.3}$$

This relation together with the fusion hierarchy of the transfer matrix leads to the T-Q relation. We then use the T-Q relation, together with some additional properties of the transfer matrix, to determine the complete set of the eigenvalues and Bethe Ansatz equations of the transfer matrix associated with the Hamiltonian (1.1) under certain constraint of the boundary parameters (see (5.16) below).

The paper is organized as follows. In Section 2, we introduce our notation and some basic ingredients. In Section 3, we derive the T-Q relation from (1.3) and the fusion hierarchy of the open XXZ chain. In section 4, some properties of the fundamental transfer matrix are obtained. By means of these properties and the T-Q relation, we in Section 5 determine the eigenvalues of the transfer matrix and the associated Bethe Ansatz equations, thus giving the complete spectrum of the Hamiltonian (1.1) under the constraint (5.16) of the boundary parameters. We summarize our conclusions in Section 6. Some detailed technical calculations are given in Appendices A-C.

2 Fundamental transfer matrix

Let us fix τ such that $\mathrm{Im}(\tau) > 0$ and a generic complex number η. Introduce the following elliptic functions

$$\theta\left[\begin{array}{c} a \\ b \end{array}\right](u,\tau) = \sum_{m=-\infty}^{\infty} \exp\left\{i\pi\left[(m+a)^2\tau + 2(m+a)(u+b)\right]\right\}, \tag{2.1}$$

$$\sigma(u) = \theta\left[\begin{array}{c} \frac{1}{2} \\ \frac{1}{2} \end{array}\right](u,\tau), \quad \zeta(u) = \frac{\partial}{\partial u}\left\{\ln\sigma(u)\right\}. \tag{2.2}$$

Among them the σ-function[1] satisfies the following identity:

$$\begin{aligned} &\sigma(u+x)\sigma(u-x)\sigma(v+y)\sigma(v-y) - \sigma(u+y)\sigma(u-y)\sigma(v+x)\sigma(v-x) \\ &\quad = \sigma(u+v)\sigma(u-v)\sigma(x+y)\sigma(x-y), \end{aligned} \tag{2.3}$$

[1] Our σ-function is the ϑ-function $\vartheta_1(u)$ [7]. It has the following relation with the *Weierstrassian* σ-function if denoted it by $\sigma_w(u)$: $\sigma_w(u) \propto e^{\eta_1 u^2}\sigma(u)$, $\eta_1 = \pi^2(\frac{1}{6} - 4\sum_{n=1}^{\infty}\frac{nq^{2n}}{1-q^{2n}})$ and $q = e^{i\tau}$.

which will be useful in deriving equations in the following.

The well-known eight-vertex model R-matrix $R(u) \in \mathrm{End}(\mathbb{C}^2 \otimes \mathbb{C}^2)$ is given by

$$R(u) = \begin{pmatrix} a(u) & & & d(u) \\ & b(u) & c(u) & \\ & c(u) & b(u) & \\ d(u) & & & a(u) \end{pmatrix}. \tag{2.4}$$

The non-vanishing matrix elements are [2]

$$a(u) = \frac{\theta\left[\begin{array}{c} 0 \\ \frac{1}{2} \end{array}\right](u, 2\tau)\, \theta\left[\begin{array}{c} \frac{1}{2} \\ \frac{1}{2} \end{array}\right](u+\eta, 2\tau)}{\theta\left[\begin{array}{c} 0 \\ \frac{1}{2} \end{array}\right](0, 2\tau)\, \theta\left[\begin{array}{c} \frac{1}{2} \\ \frac{1}{2} \end{array}\right](\eta, 2\tau)}, \quad b(u) = \frac{\theta\left[\begin{array}{c} \frac{1}{2} \\ \frac{1}{2} \end{array}\right](u, 2\tau)\, \theta\left[\begin{array}{c} 0 \\ \frac{1}{2} \end{array}\right](u+\eta, 2\tau)}{\theta\left[\begin{array}{c} 0 \\ \frac{1}{2} \end{array}\right](0, 2\tau)\, \theta\left[\begin{array}{c} \frac{1}{2} \\ \frac{1}{2} \end{array}\right](\eta, 2\tau)},$$

$$c(u) = \frac{\theta\left[\begin{array}{c} 0 \\ \frac{1}{2} \end{array}\right](u, 2\tau)\, \theta\left[\begin{array}{c} 0 \\ \frac{1}{2} \end{array}\right](u+\eta, 2\tau)}{\theta\left[\begin{array}{c} 0 \\ \frac{1}{2} \end{array}\right](0, 2\tau)\, \theta\left[\begin{array}{c} 0 \\ \frac{1}{2} \end{array}\right](\eta, 2\tau)}, \quad d(u) = \frac{\theta\left[\begin{array}{c} \frac{1}{2} \\ \frac{1}{2} \end{array}\right](u, 2\tau)\, \theta\left[\begin{array}{c} \frac{1}{2} \\ \frac{1}{2} \end{array}\right](u+\eta, 2\tau)}{\theta\left[\begin{array}{c} 0 \\ \frac{1}{2} \end{array}\right](0, 2\tau)\, \theta\left[\begin{array}{c} 0 \\ \frac{1}{2} \end{array}\right](\eta, 2\tau)}. \tag{2.5}$$

Here u is the spectral parameter and η is the so-called crossing parameter. The R-matrix satisfies the quantum Yang-Baxter equation

$$R_{1,2}(u_1-u_2)R_{1,3}(u_1-u_3)R_{2,3}(u_2-u_3) = R_{2,3}(u_2-u_3)R_{1,3}(u_1-u_3)R_{1,2}(u_1-u_2), \tag{2.6}$$

and the properties,

$$\text{PT-symmetry}: \quad R_{1,2}(u) = R_{2,1}(u) = R_{1,2}^{t_1 t_2}(u), \tag{2.7}$$

$$Z_2\text{-symmetry}: \quad \sigma_1^i \sigma_2^i R_{1,2}(u) = R_{1,2}(u)\sigma_1^i \sigma_2^i, \quad \text{for } i = x, y, z, \tag{2.8}$$

$$\text{Unitarity relation}: \; R_{1,2}(u)R_{2,1}(-u) = -\xi(u)\,\mathrm{id}, \quad \xi(u) = \frac{\sigma(u+\eta)\sigma(u-\eta)}{\sigma(\eta)\sigma(\eta)}, \tag{2.9}$$

$$\text{Crossing relation}: \; R_{1,2}(u) = V_1 R_{1,2}^{t_2}(-u-\eta)V_1, \quad V = -i\sigma^y. \tag{2.10}$$

Here $R_{2,1}(u) = P_{12}R_{1,2}(u)P_{12}$ with P_{12} being the usual permutation operator and t_i denotes transposition in the i-th space. Throughout this paper we adopt the standard notations: for any matrix $A \in \mathrm{End}(\mathbb{C}^2)$, A_j is an embedding operator in the tensor space $\mathbb{C}^2 \otimes \mathbb{C}^2 \otimes \cdots$, which acts as A on the j-th space and as identity on the other factor spaces; $R_{i,j}(u)$ is an embedding operator of R-matrix in the tensor space, which acts as identity on the factor spaces except for the i-th and j-th ones.

Integrable open spin chains can be constructed as follows [8]. Let us introduce a pair of K-matrices $K^-(u)$ and $K^+(u)$. The former satisfies the reflection equation (RE)

$$\begin{aligned} &R_{1,2}(u_1-u_2)K_1^-(u_1)R_{2,1}(u_1+u_2)K_2^-(u_2) \\ &\qquad = K_2^-(u_2)R_{1,2}(u_1+u_2)K_1^-(u_1)R_{2,1}(u_1-u_2), \end{aligned} \tag{2.11}$$

and the latter satisfies the dual RE [8, 9]

$$\begin{aligned} &R_{1,2}(u_2-u_1)K_1^+(u_1)\ R_{2,1}(-u_1-u_2-2\eta)\ K_2^+(u_2) \\ &\qquad = K_2^+(u_2)R_{1,2}(-u_1-u_2-2\eta)\ K_1^+(u_1)R_{2,1}(u_2-u_1). \end{aligned} \tag{2.12}$$

Then the transfer matrix $t(u)$ of the open XYZ chain with general integrable boundary terms is given by [8]

$$t(u) = tr_0\left(K_0^+(u)T_0(u)K_0^-(u)\hat{T}_0(u)\right), \tag{2.13}$$

where $T_0(u)$ and $\hat{T}_0(u)$ are the monodromy matrices

$$T_0(u) = R_{0,N}(u)\ldots R_{0,1}(u), \quad \hat{T}_0(u) = R_{1,0}(u)\ldots R_{N,0}(u), \tag{2.14}$$

and tr_0 denotes trace over the "auxiliary space" 0.

In this paper, we consider the most general solutions $K^{\mp}(u)$ [10] to the associated reflection equation and its dual,

$$K^-(u) = \frac{\sigma(2u)}{2\sigma(u)}\left\{I+\frac{c_x^{(-)}\sigma(u)e^{-i\pi u}}{\sigma(u+\frac{\tau}{2})}\sigma^x+\frac{c_y^{(-)}\sigma(u)e^{-i\pi u}}{\sigma(u+\frac{1+\tau}{2})}\sigma^y+\frac{c_z^{(-)}\sigma(u)}{\sigma(u+\frac{1}{2})}\sigma^z\right\}, \tag{2.15}$$

$$K^+(u) = K^-(-u-\eta)\big|_{\{c_l^{(-)}\}\rightarrow\{c_l^{(+)}\}}, \tag{2.16}$$

where I is the 2×2 identity matrix and the constants $\{c_l^{(\mp)}\}$ are expressed in terms of boundary parameters $\{\alpha_l^{(\mp)}\}$ as follows:

$$\begin{aligned} c_x^{(\mp)} &= e^{-i\pi(\sum_l\alpha_l^{(\mp)}-\frac{\tau}{2})}\prod_{l=1}^{3}\frac{\sigma(\alpha_l^{(\mp)}-\frac{\tau}{2})}{\sigma(\alpha_l^{(\mp)})}, \quad c_z^{(\mp)} = \prod_{l=1}^{3}\frac{\sigma(\alpha_l^{(\mp)}-\frac{1}{2})}{\sigma(\alpha_l^{(\mp)})}, \\ c_y^{(\mp)} &= e^{-i\pi(\sum_l\alpha_l^{(\mp)}-\frac{1}{2}-\frac{\tau}{2})}\prod_{l=1}^{3}\frac{\sigma(\alpha_l^{(\mp)}-\frac{1}{2}-\frac{\tau}{2})}{\sigma(\alpha_l^{(\mp)})}. \end{aligned} \tag{2.17}$$

Sklyanin has shown that the transfer matrices with different spectral parameters commute with each other: $[t(u)\,,t(v)]=0$. This ensures the integrability of the open XYZ chain. The Hamiltonian (1.1) can be expressed in terms of the transfer matrix

$$H=\frac{\sigma(\eta)}{\sigma'(0)}\left\{\frac{\partial}{\partial u}\,\ln t(u)\Big|_{u=0}-[(N-1)\zeta(\eta)+2\zeta(2\eta)]\right\}, \tag{2.18}$$

where $\sigma'(0)=\frac{\partial}{\partial u}\,\sigma(u)\big|_{u=0}$.

3 Fusion hierarchy and T-Q relation

We shall use the fusion procedure, which was first developed for R-matrices [11] and then later generalized for K-matrices [12, 13], to obtain the Baxter T-Q relation. The fused spin-$(j,\frac{1}{2})$ R-matrix ($j=\frac{1}{2},1,\frac{3}{2},\ldots$) is given by [11]

$$R_{\langle 1\ldots 2j\rangle,2j+1}(u)=P^{(+)}_{1\ldots 2j}R_{1,2j+1}(u)R_{2,2j+1}(u+\eta)\cdots R_{2j,2j+1}(u+(2j-1)\eta)P^{(+)}_{1\ldots 2j}, \tag{3.1}$$

where $P^{(+)}_{1\ldots 2j}$ is the completely symmetric projector. Following [12, 13], the fused spin-j K-matrix $K^{-}_{\langle 1\ldots 2j\rangle}(u)$ is given by

$$\begin{aligned}K^{-}_{\langle 1\ldots 2j\rangle}(u) \;&=\; P^{(+)}_{1\ldots 2j}\,\left\{K^{-}_{2j}(u)R_{2j,2j-1}(2u+\eta)K^{-}_{2j-1}(u+\eta)\right.\\ &\quad\times R_{2j,2j-2}(2u+2\eta)R_{2j-1,2j-2}(2u+3\eta)K^{-}_{2j-2}(u+2\eta)\cdots\\ &\quad\left.\times\, R_{2,1}(2u+(4j-3)\eta)K^{-}_{1}(u+(2j-1)\eta)\right\}\,P^{(+)}_{1\ldots 2j}.\end{aligned} \tag{3.2}$$

The fused spin-j K-matrix $K^{+}_{\langle 1\ldots 2j\rangle}(u)$ is given by

$$K^{+}_{\langle 1\ldots 2j\rangle}(u)=F(u|2j)\;K^{-}_{\langle 1\ldots 2j\rangle}(-u-2j\eta)\Big|_{\{c^{(-)}_l\}\rightarrow\{c^{(+)}_l\}}, \tag{3.3}$$

where the scalar functions $F(u|q)$ are given by $F(u|q)=1/(\prod_{l=1}^{q-1}\prod_{k=1}^{l}\xi(2u+l\eta+k\eta))$, for $q=1,2,\ldots$. The fused transfer matrix $t^{(j)}(u)$ constructed with a spin-j auxiliary space is given by

$$t^{(j)}(u)=tr_{1\ldots 2j}\left(K^{+}_{\langle 1\ldots 2j\rangle}(u)T_{\langle 1\ldots 2j\rangle}(u)K^{-}_{\langle 1\ldots 2j\rangle}(u)\hat{T}_{\langle 1\ldots 2j\rangle}(u+(2j-1)\eta)\right),\; j=\frac{1}{2},1,\ldots, \tag{3.4}$$

where

$$\begin{aligned}T_{\langle 1\ldots 2j\rangle}(u)\;&=\;R_{\langle 1\ldots 2j\rangle,N}(u)\ldots R_{\langle 1\ldots 2j\rangle,1}(u),\\ \hat{T}_{\langle 1\ldots 2j\rangle}(u+(2j-1)\eta)\;&=\;R_{\langle 1\ldots 2j\rangle,1}(u)\ldots R_{\langle 1\ldots 2j\rangle,N}(u).\end{aligned} \tag{3.5}$$

The transfer matrix (2.13) corresponds to the fundamental case $j=\frac{1}{2}$, i.e., $t(u)=t^{(\frac{1}{2})}(u)$. The fused transfer matrices constitute commutative families, namely,

$$\left[t^{(j)}(u),\, t^{(k)}(v)\right]=0. \tag{3.6}$$

They satisfy a so-called fusion hierarchy relation [12, 13]

$$t^{(j)}(u-(2j-1)\eta)=t^{(j-\frac{1}{2})}(u-(2j-1)\eta)t(u)-\delta(u)t^{(j-1)}(u-(2j-1)\eta),\ j=1,\frac{3}{2},\ldots. \tag{3.7}$$

In the above hierarchy, we have used the convention $t^{(0)}(u)=\mathrm{id}$. The coefficient function $\delta(u)$ can be expressed in terms of the quantum determinants of the monodromy matrices $T(u)$, $\hat{T}(u)$ and K-matrices [12, 13],

$$\delta(u)=\frac{\mathrm{Det}\left\{\mathrm{T(u)}\right\}\,\mathrm{Det}\left\{\hat{\mathrm{T}}\mathrm{(u)}\right\}\,\mathrm{Det}\left\{\mathrm{K^-(u)}\right\}\,\mathrm{Det}\left\{\mathrm{K^+(u)}\right\}}{\tilde{\rho}_{1,1}(2u-\eta)}. \tag{3.8}$$

Here $\tilde{\rho}_{1,1}(u)=\frac{\sigma(-u)\sigma(u+2\eta)}{\sigma(\eta)\sigma(\eta)}$ and the corresponding determinants are given by [13]

$$\begin{aligned}
\mathrm{Det}\left\{\mathrm{T(u)}\right\}\,\mathrm{id} &= tr_{12}\left(P^{(-)}_{12}T_1(u-\eta)T_2(u)P^{(-)}_{12}\right)=\left(\frac{\sigma(u+\eta)\sigma(u-\eta)}{\sigma(\eta)\sigma(\eta)}\right)^N\mathrm{id}, & (3.9)\\
\mathrm{Det}\left\{\hat{\mathrm{T}}\mathrm{(u)}\right\}\,\mathrm{id} &= tr_{12}\left(P^{(-)}_{12}T_1(u-\eta)T_2(u)P^{(-)}_{12}\right)=\left(\frac{\sigma(u+\eta)\sigma(u-\eta)}{\sigma(\eta)\sigma(\eta)}\right)^N\mathrm{id}, & (3.10)\\
\mathrm{Det}\left\{\mathrm{K^-(u)}\right\} &= tr_{12}\left(P^{(-)}_{12}K^-_1(u-\eta)R_{12}(2u-\eta)K^-_2(u)\right), & (3.11)\\
\mathrm{Det}\left\{\mathrm{K^+(u)}\right\} &= tr_{12}\left(P^{(-)}_{12}K^+_2(u)R_{12}(-2u-\eta)K^+_1(u-\eta)\right), & (3.12)
\end{aligned}$$

where $P^{(-)}_{12}$ is the completely antisymmetric project: $P^{(-)}_{12}=\frac{1}{2}\left(\mathrm{id}-P_{12}\right)$. Using the crossing relations of the K-matrices (see (4.9)-(4.12) below) and after a tedious calculation (for details see Appendix A), we find that the quantum determinants of the most general K-matrices $K^{\pm}(u)$ given by (2.15) and (2.16) respectively are

$$\begin{aligned}
\mathrm{Det}\left\{\mathrm{K^-(u)}\right\} &= \frac{\sigma(2u-2\eta)}{\sigma(\eta)}\prod_{l=1}^{3}\frac{\sigma(\alpha_l^{(-)}+u)\sigma(\alpha_l^{(-)}-u)}{\sigma(\alpha_l^{(-)})\sigma(\alpha_l^{(-)})}, & (3.13)\\
\mathrm{Det}\left\{\mathrm{K^+(u)}\right\} &= \frac{\sigma(2u+2\eta)}{\sigma(\eta)}\prod_{l=1}^{3}\frac{\sigma(u+\alpha_l^{(+)})\sigma(u-\alpha_l^{(+)})}{\sigma(\alpha_l^{(+)})\sigma(\alpha_l^{(+)})}. & (3.14)
\end{aligned}$$

Substituting (3.9)-(3.14) into (3.8), one has that

$$\begin{aligned}
\delta(u)=&\left\{\frac{\sigma(u+\eta)\sigma(u-\eta)}{\sigma(\eta)\sigma(\eta)}\right\}^{2N}\frac{\sigma(2u-2\eta)\sigma(2u+2\eta)}{\sigma(2u-\eta)\sigma(2u+\eta)}\\
&\times\prod_{\gamma=\pm}\prod_{l=1}^{3}\frac{\sigma(u+\alpha_l^{(\gamma)})\sigma(u-\alpha_l^{(\gamma)})}{\sigma(\alpha_l^{(\gamma)})\sigma(\alpha_l^{(\gamma)})}.
\end{aligned}\tag{3.15}$$

For generic η, the fusion hierarchy does not truncate (c.f. the roots of unity case in the trigonometric limit [14, 15]). Hence $\{t^{(j)}(u)\}$ constitute an infinite hierarchy, namely, j taking values $\frac{1}{2}, 1, \frac{3}{2}, \ldots$. The commutativity (3.6) of the fused transfer matrices $\{t^{(j)}(u)\}$ and the fusion relation (3.7) imply that the corresponding eigenvalue of the transfer matrix $t^{(j)}(u)$, denoted by $\Lambda^{(j)}(u)$, satisfies the following hierarchy relation

$$\begin{aligned}\Lambda^{(j)}(u+\eta-2j\eta) &= \Lambda^{(j-\frac{1}{2})}(u-2(j-\frac{1}{2})\eta)\,\Lambda(u)-\delta(u)\,\Lambda^{(j-1)}(u-\eta-2(j-1)\eta),\\ & j=1,\frac{3}{2},\ldots .\end{aligned} \tag{3.16}$$

Here we have used the convention $\Lambda(u)=\Lambda^{(\frac{1}{2})}(u)$ and $\Lambda^{(0)}(u)=1$. Dividing both sides of (3.16) by $\Lambda^{(j-\frac{1}{2})}(u-2(j-\frac{1}{2})\eta)$, we have

$$\Lambda(u)=\frac{\Lambda^{(j)}(u+\eta-2j\eta)}{\Lambda^{(j-\frac{1}{2})}(u-2(j-\frac{1}{2})\eta)}+\delta(u)\,\frac{\Lambda^{(j-1)}(u-\eta-2(j-1)\eta)}{\Lambda^{(j-\frac{1}{2})}(u-2(j-\frac{1}{2})\eta)}. \tag{3.17}$$

We now consider the limit $j\to\infty$. We make the fundamental assumption (1.3) (in particular, that the limit exists), which implies for the corresponding eigenvalues

$$\bar{Q}(u)=\lim_{j\longrightarrow+\infty}\Lambda^{(j)}(u-2j\eta), \tag{3.18}$$

where we have used the same notation for the operator $\bar{Q}$ and its eigenvalues (c.f. Eq.(1.3)). It follows from (3.17) that

$$\Lambda(u)=\frac{\bar{Q}(u+\eta)}{\bar{Q}(u)}+\delta(u)\,\frac{\bar{Q}(u-\eta)}{\bar{Q}(u)}. \tag{3.19}$$

Assuming the function $\bar{Q}(u)$ has the decomposition $\bar{Q}(u)=f(u)Q(u)$ with

$$Q(u)=\prod_{j=1}^{M}\sigma(u-u_j)\sigma(u+u_j+\eta), \tag{3.20}$$

where M is certain non-negative integer and $\{u_j\}$ are some parameters which will be specified later (see (5.17) and (5.19) below), then Eq. (3.19) becomes

$$\Lambda(u)=H_1(u)\,\frac{Q(u+\eta)}{Q(u)}+H_2(u)\,\frac{Q(u-\eta)}{Q(u)}. \tag{3.21}$$

Here $H_1(u)=\frac{f(u+\eta)}{f(u)}$ and $H_2(u)=\delta(u)\,\frac{f(u-\eta)}{f(u)}$. It is easy to see that the functions $\{H_i(u)|i=1,2\}$ satisfy the relation

$$H_1(u-\eta)H_2(u)=\delta(u) \tag{3.22}$$

with $\delta(u)$ given by (3.15).

In summary, the eigenvalue $\Lambda(u)$ of the fundamental transfer matrix $t(u)$ (2.13) has the decomposition form (3.21), where the coefficient functions $\{H_i(u)\}$ satisfy the constraint (3.22). In the following, we shall use certain properties of the eigenvalue $\Lambda(u)$ derived from the transfer matrix to determine the functions $\{H_i(u)\}$ and therefore the eigenvalue $\Lambda(u)$.

4 Properties of the fundamental transfer matrix

Here we will derive five properties of the fundamental transfer matrix $t(u)$, which together with the T-Q relation (3.21) enable us to determine the functions $\{H_i(u)\}$.

In addition to the Riemann identity (2.3), the σ-function enjoys the following identity:

$$\sigma(2u) = \frac{2\sigma(u)\sigma(u+\frac{1}{2})\sigma(u+\frac{\tau}{2})\sigma(u-\frac{1}{2}-\frac{\tau}{2})}{\sigma(\frac{1}{2})\sigma(\frac{\tau}{2})\sigma(-\frac{1}{2}-\frac{\tau}{2})}, \tag{4.1}$$

$$\sigma(u+1) = -\sigma(u), \quad \sigma(u+\tau) = -e^{-2i\pi(u+\frac{\tau}{2})}\sigma(u). \tag{4.2}$$

Moreover, from the definition of the elliptic function (2.1), one may show that

$$\theta\left[\begin{array}{c}0\\ \frac{1}{2}\end{array}\right](u+\tau,2\tau) = e^{-i\pi(u+\frac{1}{2}+\frac{\tau}{2})}\,\theta\left[\begin{array}{c}\frac{1}{2}\\ \frac{1}{2}\end{array}\right](u,2\tau), \tag{4.3}$$

$$\theta\left[\begin{array}{c}\frac{1}{2}\\ \frac{1}{2}\end{array}\right](u+\tau,2\tau) = e^{-i\pi(u+\frac{1}{2}+\frac{\tau}{2})}\,\theta\left[\begin{array}{c}0\\ \frac{1}{2}\end{array}\right](u,2\tau). \tag{4.4}$$

The property (4.1) of the σ-function implies that the matrix elements of the K-matrices $K^{\mp}(u)$ given by (2.15)-(2.16) are analytic functions of u. Thus the commutativity of the transfer matrix $t(u)$ and the analyticity of the R-matrix and K-matrices lead to the following analytic property:

$$\text{The eigenvalue of } t(u) \text{ is an analytic function of } u \text{ at finite } u. \tag{4.5}$$

The quasi-periodicity of the elliptic functions, (4.2)-(4.4), allows one to derive the following properties of the R-matrix and K-matrices:

$$\begin{aligned}
R_{1,2}(u+1) &= -\sigma_1^z R_{1,2}(u)\sigma_1^z = -\sigma_2^z R_{1,2}(u)\sigma_2^z, \quad K^{\mp}(u+1) = -\sigma^z K^{\mp}(u)\sigma^z,\\
R_{1,2}(u+\tau) &= -e^{-2i\pi(u+\frac{\eta}{2}+\frac{\tau}{2})}\sigma_1^x R_{1,2}(u)\sigma_1^x = -e^{-2i\pi(u+\frac{\eta}{2}+\frac{\tau}{2})}\sigma_2^x R_{1,2}(u)\sigma_2^x,\\
K^-(u+\tau) &= -e^{-2i\pi(3u+\frac{3}{2}\tau)}\sigma^x K^-(u)\sigma^x,\\
K^+(u+\tau) &= -e^{-2i\pi(3u+3\eta+\frac{3}{2}\tau)}\sigma^x K^+(u)\sigma^x.
\end{aligned}$$

From these relations one obtains the quasi-periodic properties of $t(u)$,

$$t(u+1) = t(u), \quad t(u+\tau) = e^{-2i\pi(N+3)(2u+\eta+\tau)}\, t(u). \tag{4.6}$$

The initial conditions of the R-matrix $R_{12}(0) = P_{12}$ and K-matrices: $K^-(0) = \text{id}$, $trK^+(0) = \sigma(2\eta)/\sigma(\eta)$, imply that the initial condition of the fundamental transfer matrix $t(u)$ is given by

$$t(u)|_{u=0} = \frac{\sigma(2\eta)}{\sigma(\eta)} \times \text{id}. \tag{4.7}$$

The identity

$$\frac{\sigma(u)}{\sigma(\frac{\tau}{2})} = \frac{\theta\begin{bmatrix} 0 \\ \frac{1}{2} \end{bmatrix}(u, 2\tau)\; \theta\begin{bmatrix} \frac{1}{2} \\ \frac{1}{2} \end{bmatrix}(u, 2\tau)}{\theta\begin{bmatrix} 0 \\ \frac{1}{2} \end{bmatrix}(\frac{\tau}{2}, 2\tau)\; \theta\begin{bmatrix} \frac{1}{2} \\ \frac{1}{2} \end{bmatrix}(\frac{\tau}{2}, 2\tau)},$$

suggests the semi-classical property of the R-matrix $\lim_{\eta\to 0}\{\sigma(\eta)R_{12}(u)\} = \sigma(u)\,\text{id}$. This enables us to derive the semi-classical property of $t(u)$,

$$\lim_{\eta\to 0}\{\sigma^{2N}(\eta)t(u)\} = \sigma^{2N}(u)\lim_{\eta\to 0}\{tr(K^+(u)K^-(u))\} \times \text{id}. \tag{4.8}$$

Now, we derive the crossing relation of $t(u)$. For this purpose, we introduce

$$\bar{K}_1^-(u) = tr_2\left(P_{12}R_{12}(-2u-2\eta)\{K_2^-(u)\}^{t_2}\right), \tag{4.9}$$

$$\bar{K}_1^+(u) = tr_2\left(P_{12}R_{12}(2u)\{K_2^+(u)\}^{t_2}\right). \tag{4.10}$$

Through a straightforward calculation (see Appendix A for details), we find

$$\bar{K}^-(u) = -\frac{\sigma(2u)}{\sigma(\eta)}\sigma^y K^-(-u-\eta)\sigma^y \equiv f_-(u)VK^-(-u-\eta)V, \tag{4.11}$$

$$\bar{K}^+(u) = \frac{\sigma(2u+2\eta)}{\sigma(\eta)}\sigma^y K^+(-u-\eta)\sigma^y \equiv f_+(u)VK^+(-u-\eta)V, \tag{4.12}$$

where the 2×2 matrix V is given in (2.10), $f_-(u) = \frac{\sigma(2u)}{\sigma(\eta)}$ and $f_+(u) = -\frac{\sigma(2u+2\eta)}{\sigma(\eta)}$. The PT-symmetry (2.7) and crossing relation (2.10) of the R-matrix implies

$$\begin{aligned}
T_0^{t_0}(-u-\eta) &= (R_{0,N}(-u-\eta)\ldots R_{0,1}(-u-\eta))^{t_0} \\
&\overset{(2.10)}{=} (-1)^{N-1}\left(V_0\, R_{0,N}^{t_N}(u)\ldots R_{0,1}^{t_1}(u)\, V_0\right)^{t_0} \\
&= (-1)^{N-1}\left(V_0\,\{R_{0,N}(u)\ldots R_{0,1}(u)\}^{t_1\ldots t_N}\, V_0\right)^{t_0} \\
&= (-1)^{N-1}\, V_0\,\{R_{0,N}(u)\ldots R_{0,1}(u)\}^{t_0\, t_1\ldots t_N}\, V_0 \\
&\overset{(2.7)}{=} (-1)^{N-1}\, V_0 R_{0,1}(u)\ldots R_{0,N}(u)\, V_0 \overset{(2.7)}{=} (-1)^{N-1}V_0\hat{T}_0(u)V_0,
\end{aligned} \tag{4.13}$$

Similarly, we have another "duality relations" between the monodromoy matrices $T(u)$ and $\hat{T}(u)$,

$$\hat{T}_0^{t_0}(-u-\eta) = (-1)^{N-1} V_0\, T_0(u)\, V_0. \tag{4.14}$$

The crossing relations of the K-matrices (4.11) and (4.12), and the "duality relations" (4.13) and (4.14), imply that

$$\begin{aligned}
t(-u-\eta) &= tr_0\left(K_0^+(-u-\eta)T_0(-u-\eta)K_0^-(-u-\eta)\hat{T}_0(-u-\eta)\right)\\
&= tr_0\left(\left\{K_0^+(-u-\eta)T_0(-u-\eta)\right\}^{t_0}\left\{K_0^-(-u-\eta)\hat{T}_0(-u-\eta)\right\}^{t_0}\right)\\
&= tr_0\left(T_0^{t_0}(-u-\eta)(K_0^+(-u-\eta))^{t_0}\hat{T}_0^{t_0}(-u-\eta)(K_0^-(-u-\eta))^{t_0}\right)\\
&\overset{(4.13),(4.14)}{=} tr_0\left(\hat{T}_0(u)\left\{V_0(K_0^+(-u-\eta))^{t_0}V_0\right\}T_0(u)\left\{V_0(K_0^-(-u-\eta))^{t_0}V_0\right\}\right)\\
&\overset{(4.11),(4.12)}{=} tr_0\left(\hat{T}_0(u)(\bar{K}_0^+(u))^{t_0}T_0(u)(\bar{K}_0^-(u))^{t_0}\right)/f_+(u)f_-(u)\\
&\overset{(4.9),(4.10)}{=} \frac{tr_0tr_1tr_2\Big(\hat{T}_0(u)P_{01}R_{0,1}(2u)K_1^+(u)T_0(u)P_{02}R_{0,2}(-2u-2\eta)K_2^-(u)\Big)}{f_+(u)f_-(u)}\\
&= \frac{tr_0tr_1tr_2\Big(P_{01}\hat{T}_1(u)R_{0,1}(2u)T_0(u)P_{02}R_{0,2}(-2u-2\eta)K_2^-(u)K_1^+(u)\Big)}{f_+(u)f_-(u)}\\
&= \frac{tr_0tr_1tr_2\Big(K_1^+(u)T_1(u)P_{01}R_{0,1}(2u)P_{02}R_{0,2}(-2u-2\eta)K_2^-(u)\hat{T}_1(u)\Big)}{f_+(u)f_-(u)}.
\end{aligned} \tag{4.15}$$

In deriving the second last equality of the above equation, we have used the relation, $\hat{T}_1(u)R_{0,1}(2u)T_0(u) = T_0(u)R_{0,1}(2u)\hat{T}_1(u)$, which is a simple consequence of the quantum Yang-Baxter equation (2.6). Then, let us consider

$$\begin{aligned}
&tr_0tr_2\left(P_{01}R_{0,1}(2u)P_{02}R_{0,2}(-2u-2\eta)K_2^-(u)\right)/f_+(u)f_-(u)\\
&\quad= tr_0\left(P_{01}R_{0,1}(2u)tr_2\left\{P_{02}R_{0,2}(-2u-2\eta)K_2^-(u)\right\}\right)/f_+(u)f_-(u)\\
&\quad\overset{(4.9)}{=} tr_0\left(P_{01}R_{0,1}(2u)\left\{\bar{K}_0^-(u)\right\}^{t_0}\right)/f_+(u)f_-(u)\\
&\quad\overset{(4.11)}{=} tr_0\left(V_0P_{01}R_{0,1}(2u)V_0\left\{K_0^-(-u-\eta)\right\}^{t_0}\right)/f_+(u)\\
&\quad\overset{(2.8)}{=} tr_0\left(V_1P_{01}R_{0,1}(2u)V_1\left\{K_0^-(-u-\eta)\right\}^{t_0}\right)/f_+(u)\\
&\quad\overset{(4.9)}{=} V_1\bar{K}_1^-(-u-\eta)V_1/f_+(u) \overset{(4.11)}{=} \frac{f_-(-u-\eta)}{f+(u)}K_1^-(u) = K_1^-(u)
\end{aligned}$$

Substituting the above equation into (4.15), we have the following crossing relation of $t(u)$:

$$t(-u-\eta) = tr_1\left(K_1^+(u)T_1(u)K_1^-(u)\hat{T}_1(u)\right) = t(u). \tag{4.16}$$

We remark that our above proof of the crossing relation (4.16) generalizes the previous proofs given in [16].

5 Eigenvalues and Bethe Ansatz equations

It follows from (4.5)-(4.8) and (4.16) that the eigenvalue $\Lambda(u)$, as a function of u, has the following properties,

$$\text{Analyticity :} \quad \Lambda(u) \text{ is an analytic function of } u \text{ at finite } u. \tag{5.1}$$

$$\text{Quasi-Periodicity :} \quad \Lambda(u+1)=\Lambda(u), \quad \Lambda(u+\tau)=e^{-2i\pi(N+3)(2u+\eta+\tau)}\Lambda(u), \tag{5.2}$$

$$\text{Crossing symmetry :} \quad \Lambda(-u-\eta)=\Lambda(u), \tag{5.3}$$

$$\text{Initial condition :} \quad \Lambda(0)=\frac{\sigma(2\eta)}{\sigma(\eta)}, \tag{5.4}$$

$$\text{Semi-classic property :} \quad \lim_{\eta\to 0}\left\{\sigma^{2N}(\eta)\Lambda(u)\right\}=\sigma^{2N}(u)\lim_{\eta\to 0}\left\{tr(K^+(u)K^-(u))\right\}. \tag{5.5}$$

The T-Q relations (3.21) and (3.22), together with the above properties (5.1)-(5.5), can be used to determine $\{H_i(u)\}$ and the eigenvalues of the fundamental transfer matrix.

For this purpose, we define 6 *discrete* parameters $\{\epsilon_l^{(\gamma)}=\pm 1|\gamma=\pm,\, l=1,2,3\}$ and fix $\epsilon_1^{(-)}=+1$ in the following. Associated with $\{\epsilon_l^{(\gamma)}\}$, we introduce

$$\begin{aligned} H_1^{(\pm)}(u|\{\epsilon_l^{(\gamma)}\}) &= \frac{\sigma^{2N}(u)\sigma(2u)}{\sigma^{2N}(\eta)\sigma(2u+\eta)}\prod_{\gamma=\pm}\prod_{l=1}^{3}\frac{\sigma(u+\eta\pm\epsilon_l^{(\gamma)}\alpha_l^{(\gamma)})}{\sigma(\epsilon_l^{(\gamma)}\alpha_l^{(\gamma)})}, &(5.6)\\ H_2^{(\pm)}(u|\{\epsilon_l^{(\gamma)}\}) &= \frac{\sigma^{2N}(u+\eta)\sigma(2u+2\eta)}{\sigma^{2N}(\eta)\sigma(2u+\eta)}\prod_{\gamma=\pm}\prod_{l=1}^{3}\frac{\sigma(u\mp\epsilon_l^{(\gamma)}\alpha_l^{(\gamma)})}{\sigma(\epsilon_l^{(\gamma)}\alpha_l^{(\gamma)})}. &(5.7)\end{aligned}$$

One may readily check that the functions $H_1^{(\pm)}(u|\{\epsilon_l^{(\gamma)}\})$ and $H_2^{(\pm)}(u|\{\epsilon_l^{(\gamma)}\})$ indeed satisfy (3.22), namely,

$$H_1^{(\pm)}(u-\eta|\{\epsilon_l^{(\gamma)}\})H_2^{(\pm)}(u|\{\epsilon_l^{(\gamma)}\})=\delta(u). \tag{5.8}$$

The general solution to (3.22) can be written as follows:

$$H_1(u)=H_1^{(\pm)}(u|\{\epsilon_l^{(\gamma)}\})\,g_1(u), \quad H_2(u)=H_2^{(\pm)}(u|\{\epsilon_l^{(\gamma)}\})\,g_2(u), \tag{5.9}$$

where $\{g_i(u)\}$ satisfy the following relations,

$$g_1(u-\eta)g_2(u)=1, \quad g_1(u+1)=g_1(u), \quad g_2(u+1)=g_2(u). \tag{5.10}$$

The solutions to (5.10) have the following form,

$$g_1(u) = \lambda \frac{\prod_{j=1}^{N_2} \sigma(u - u_j^+)}{\prod_{j=1}^{N_1} \sigma(u - u_j^-)}, \quad g_2(u) = \frac{1}{\lambda} \frac{\prod_{j=1}^{N_1} \sigma(u - u_j^- - \eta)}{\prod_{j=1}^{N_2} \sigma(u - u_j^+ - \eta)}, \tag{5.11}$$

where N_1 and N_2 are integers such that N_1, $N_2 \geq 0$, and λ is an non-zero constant. In the above equation, we assume that $u_j^- \neq \mp\epsilon_l^{(\gamma)}\alpha_l^{(\gamma)} - \eta$ and $u_j^+ \neq \mp\epsilon_{l'}^{(\gamma')}\alpha_{l'}^{(\gamma')} - \eta$, otherwise the corresponding factors in $g_i(u)$ make transitions among $\{H_1^{(\pm)}(u|\{\epsilon_l^{(\gamma)}\})\}$ ($\{H_2^{(\pm)}(u|\{\epsilon_l^{(\gamma)}\})\}$ respectively). Then the analyticity of $\Lambda(u)$ (5.1) requires that $g_1(u)$ and $g_2(u)$ have common poles; i.e., $N_1 = N_2$, and $u_j^- = u_{j'}^+ + \eta$. This means

$$g_1(u) = \lambda \prod_{j=1}^{N_1} \frac{\sigma(u - u_j^- + \eta)}{\sigma(u - u_j^-)}, \quad g_2(u) = \frac{1}{\lambda} \prod_{j=1}^{N_1} \frac{\sigma(u - u_j^- - \eta)}{\sigma(u - u_j^-)}. \tag{5.12}$$

Since $H_2^{(\pm)}(u|\{\epsilon_l^{(\gamma)}\}) = H_1^{(\pm)}(-u-\eta|\{\epsilon_l^{(\gamma)}\})$, the crossing symmetry of $\Lambda(u)$ (5.3) implies that $H_2(u) = H_1(-u-\eta)$. Hence, N_1 is even and

$$g_1(u) = \lambda \prod_{j=1}^{\frac{N_1}{2}} \frac{\sigma(u - u_j^- + \eta)\sigma(u + u_j^- + 2\eta)}{\sigma(u - u_j^-)\sigma(u + u_j^- + \eta)}, \tag{5.13}$$

$$g_2(u) = \lambda \prod_{j=1}^{\frac{N_1}{2}} \frac{\sigma(u - u_j^- - \eta)\sigma(u + u_j^-)}{\sigma(u - u_j^-)\sigma(u + u_j^- + \eta)}, \quad \lambda = \pm 1. \tag{5.14}$$

This is equivalent to having additional Bethe roots; and the corresponding factors, except λ, can be absorbed into those of $Q(u)$ (3.20). Moreover the initial condition (5.4) implies $\lambda = +1$. Therefore the eigenvalues of the transfer matrix take the following forms:

$$H_1^{(\pm)}(u|\{\epsilon_l^{(\gamma)}\}) \frac{Q(u+\eta)}{Q(u)} + H_2^{(\pm)}(u|\{\epsilon_l^{(\gamma)}\}) \frac{Q(u-\eta)}{Q(u)}. \tag{5.15}$$

In the above expression, we still have an unknown non-negative integer M defined in (3.20) to be fixed. Moreover, $\Lambda(u)$ must fulfill the properties (5.2) and (5.5). This provides the following constraint to the boundary parameters $\{\alpha_l^{(\gamma)}\}$:

$$\sum_{\gamma=\pm} \sum_{l=1}^{3} \epsilon_l^{(\gamma)} \alpha_l^{(\gamma)} = k\eta \mod(1), \qquad \prod_{\gamma=\pm} \prod_{l=1}^{3} \epsilon_l^{(\gamma)} = -1, \tag{5.16}$$

where k is an integer such that $|k| \leq N-1$ and $N-1+k$ being even, and yields two different values $M^{(\pm)}$ for M in (3.20), corresponding respectively to $H_i^{(\pm)}(u|\{\epsilon_l^{(\gamma)}\})$,

$$M^{(\pm)} = \frac{1}{2}(N - 1 \mp k). \tag{5.17}$$

The proof of the above constraint is relegated to Appendix B.

Finally, we have that if the boundary parameters $\{\alpha_l^{(\gamma)}\}$ satisfy any of the constraints (5.16), the eigenvalues of the fundamental transfer matrix $t(u)$ are given by

$$\Lambda^{(\pm)}(u) \quad = \quad H_1^{(\pm)}(u|\{\epsilon_l^{(\gamma)}\})\frac{Q^{(\pm)}(u+\eta)}{Q^{(\pm)}(u)} + H_2^{(\pm)}(u|\{\epsilon_l^{(\gamma)}\})\frac{Q^{(\pm)}(u-\eta)}{Q^{(\pm)}(u)}, \tag{5.18}$$

where $Q^{(\pm)}(u) = \prod_{j=1}^{M^{(\pm)}} \sigma(u - u_j^{(\pm)})\sigma(u + u_j^{(\pm)} + \eta)$ and the parameters $\{u_j^{(\pm)}\}$ respectively satisfy the Bethe Ansatz equations,

$$\frac{H_2^{(\pm)}(u_j^{(\pm)}|\{\epsilon_l^{(\gamma)}\})}{H_1^{(\pm)}(u_j^{(\pm)}|\{\epsilon_l^{(\gamma)}\})} = -\frac{Q^{(\pm)}(u_j^{(\pm)}+\eta)}{Q^{(\pm)}(u_j^{(\pm)}-\eta)}, \qquad j = 1, \ldots, M^{(\pm)}. \tag{5.19}$$

Indeed one can verify that both $\Lambda^{(\pm)}(u)$ given by (5.18) have the desirable properties (5.1)-(5.5) provided that the constraint (5.16) and the Bethe Ansatz equations (5.19) are satisfied. In the trigonometric limit $\tau \to +i\infty$, we recover the results in [5] (for details see Appendix C). The completeness [17, 5] of the eigenvalues $\{\Lambda^{(\pm)}(u)\}$ in the trigonometric case suggests that for a given set of bulk and boundary parameters satisfying the constraint (5.16), the eigenvalues $\Lambda^{(-)}(u)$ and $\Lambda^{(+)}(u)$ *together* constitute the complete set of eigenvalues of the transfer matrix $t(u)$ of the open XYZ spin chain.

Therefore the complete set of the energy eigenvalues $E^{(\pm)}$ of the Hamiltonian (1.1), when the boundary parameters satisfy the constraint (5.16), are respectively given by

$$E^{(\pm)} = \frac{\sigma(\eta)}{\sigma'(0)}\left\{2\sum_{j=1}^{M^{(\pm)}}\Big(\zeta(u_j^{(\pm)}) - \zeta(u_j^{(\pm)}+\eta)\Big) + (N-1)\zeta(\eta) + \sum_{\gamma=\pm}\sum_{l=1}^{3}\zeta(\mp\epsilon_l^{(\gamma)}\alpha_l^{(\gamma)})\right\}, \tag{5.20}$$

where the parameters $\{u_j^{(\pm)}\}$ respectively satisfy the Bethe Ansatz equations (5.19).

Some remarks are in order. Firstly, in [18] a generalized algebraic Bethe Ansatz [19] was used to diagonalize the open XYZ spin chain when boundary parameters satisfying a constraint. However, only *partial* eigenvalues of transfer matrix corresponding to our $\Lambda^{(+)}(u)$ were obtained there and it is not clear whether the approach in [18] can give all the eigenvalues of the transfer matrix. (See also [20], where partial eigenvalues of the transfer matrix of the open XXZ spin chain were obtained.) Indeed, it is found in this paper that both $\Lambda^{(\pm)}(u)$ are needed to constitute a complete set of eigenvalues. This implies that two sets of Bethe Ansatz equation (5.19) and therefore presumably two pseudo-vacua are required. Unfortunately, it is not yet clear how to construct the second pseudo-vacuum in

the generalized algebraic Bethe Ansatz approach. Secondly, when the crossing parameter η is equal to $\frac{1}{p+1}$ with p being a non-negative integer (i.e. roots of unity case), the corresponding fusion hierarchy truncates as in the trigonometric case [14], and one may generalize the method developed in [15] to obtain the corresponding functional relations obeyed by the transfer matrices and therefore the eigenvalues of the fundamental transfer matrix $t(u)$. If the boundary parameters satisfy the constraint (5.16), the complete set of eigenvalues and the associated Bethe Ansatz equations, in the roots of unity case, are expected to be *still* given by (5.18) and (5.19) respectively. Thirdly, it would be interesting to determine the conditions for which the limit (1.3) exists. We have seen that (5.18)-(5.19) solve the open XYZ chain with generic values of η if the constraint (5.16) is satisfied. This suggests that, for generic values of η, the constraint (5.16) may be a necessary condition for the existence of the limit (1.3). It would be interesting to explicitly evaluate the Q-operator directly from Eq. (1.3).

6 Conclusions

We have argued that the Baxter's Q-operator for the open XYZ chain is given by the $j \to \infty$ limit of the transfer matrix with spin-j auxiliary space. This together with the fusion hierarchy leads to the Baxter's T-Q relations (3.21) and (3.22). These T-Q relations, together with the additional properties (5.1)-(5.5), enable us to successfully determine the eigenvalues (5.18) of the fundamental transfer matrix and the associated Bethe Ansatz equations (5.19). For a given set of bulk and boundary parameters satisfying the constraint (5.16), the eigenvalues $\Lambda^{(-)}(u)$ and $\Lambda^{(+)}(u)$ *together* constitute the complete set of eigenvalues of the fundamental transfer matrix $t(u)$, which leads to the complete spectrum (5.20) of the Hamiltonian (1.1). Our derivation for the Q-operator and associated T-Q relation can be applied to other models which share sl_2-like fusion rule. Moreover, it would be interesting to generalize our method to integrable models associated with higher rank algebras [21, 22, 23].

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Appendix A: Determinants and crossing relations

In this appendix, we compute the determinants (3.11) and (3.12) of the K-matrices. In so doing, we will also prove the crossing relations (4.11) and (4.12).

One rewrites $K^-(u)$ in (2.15) as

$$K^-(u) = \sum_{\alpha=0}^{3} f_\alpha(u)\sigma^\alpha, \quad \sigma^0 = I,\, \sigma^1 = \sigma^x,\, \sigma^2 = \sigma^y,\, \sigma^3 = \sigma^z.$$

It is easy checked that the coefficient function $\{f_\alpha(u)\}$ satisfy

$$f_0(-u) = f_0(u), \qquad f_i(-u) = -f_i(u), \quad \text{for } i = 1, 2, 3.$$

The above parity relations lead to the following unitarity relation of $K^-(u)$

$$K^-(u)K^-(-u) = \Delta_2(u) \times \mathrm{id}, \quad \Delta_2(u) = \sum_{\alpha=0}^{3} f_\alpha(u) f_\alpha(-u). \tag{A.1}$$

From the expression (2.15) of $K^-(u)$ and after direct calculation, we find that

$$\Delta_2(u) = \prod_{l=1}^{3} \frac{\sigma(\alpha_l^{(-)} + u)\sigma(\alpha_l^{(-)} - u)}{\sigma(\alpha_l^{(-)})\sigma(\alpha_l^{(-)})}. \tag{A.2}$$

We now follow a method similar to that developed in [24]. Noting $R_{1,2}(-\eta) = -2P_{12}^{(-)}$ and PT-symmetry (2.7) of the R-matrix, the reflection equation (2.11), when $u_1 = u$, $u_2 = u+\eta$, reads

$$P_{12}^{(-)} K_1^-(u) R_{1,2}(2u+\eta) K_2^-(u+\eta) = K_2^-(u+\eta) R_{1,2}(2u+\eta) K_1^-(u) P_{12}^{(-)}.$$

Since the dimension of the image of $P_{12}^{(-)}$ is equal to one, the above equation becomes

$$\begin{aligned} K_2^-(u+\eta) R_{1,2}(2u+\eta) K_1^-(u) P_{12}^{(-)} &= P_{12}^{(-)} K_1^-(u) R_{1,2}(2u+\eta) K_2^-(u+\eta) P_{12}^{(-)} \\ &= tr_{12}\left(P_{12}^{(-)} K_1^-(u) R_{1,2}(2u+\eta) K_2^-(u+\eta)\right) P_{12}^{(-)} \\ &\overset{(3.11)}{=} \mathrm{Det}\{K^-(u+\eta)\}\, P_{12}^{(-)}. \end{aligned} \tag{A.3}$$

It is well-known that the completely anti-symmetric vector with unit normal in $\mathbb{C}^2 \otimes \mathbb{C}^2$ is

$$\frac{1}{\sqrt{2}} \left(|1\rangle \otimes |2\rangle - |2\rangle \otimes |1\rangle\right) = (\mathrm{id} \otimes V) \left(\frac{1}{\sqrt{2}} \sum_{i=1}^{2} |i\rangle \otimes |i\rangle\right), \tag{A.4}$$

where $\{|1\rangle, |2\rangle\}$ are the orthnormal basis of $\mathbb{C}^2$. Acting both sides of (A.3) on the vector (A.4) and after straightforward calculating, we find that (A.3) is indeed equivalent to

$$\bar{K}^-(u) = \mathrm{Det}\{K^-(u+\eta)\}\left\{VK^-(u+\eta)V\right\}^{-1}.$$

Using (A.1), we have

$$\bar{K}^-(u) = \frac{\mathrm{Det}\{K^-(u+\eta)\}}{\Delta_2(u+\eta)}VK^-(-u-\eta)V. \tag{A.5}$$

Taking trace of both sides of (A.5), we have, for the L.H.S. of the resulting relation,

$$\begin{aligned}\text{L.H.S.} &= tr\left(\bar{K}^-(u)\right) \overset{(4.9)}{=} tr_{12}\left(P_{12}R_{1,2}(-2u-2\eta)\{K_2^-(u)\}^{t_2}\right)\\ &= tr_2\left(tr_1\left\{P_{12}R_{1,2}(-2u-2\eta)\right\}\{K_2^-(u)\}^{t_2}\right)\\ &= \left(a(-2u-2\eta)+c(-2u-2\eta)\right)tr_2\left(K_2^-(u)\right)\\ &= \left(a(-2u-2\eta)+c(-2u-2\eta)\right)\frac{\sigma(2u)}{\sigma(u)}\\ &= -\frac{\sigma(2u)\sigma(2u+2\eta)}{\sigma(\eta)\sigma(u+\eta)}.\end{aligned} \tag{A.6}$$

In the above deriving, we have used the following relations:

$$\begin{aligned}tr_1\left(P_{12}R_{1,2}(u)\right) &= (a(u)+c(u))\times \mathrm{id},\\ a(-2u-2\eta)+c(-2u-2\eta) &= -\frac{\sigma(2u+2\eta)\sigma(u)}{\sigma(\eta)\sigma(u+\eta)},\end{aligned}$$

which can be obtained from (2.3)-(2.5), and the following identities of the elliptic functions:

$$\begin{aligned}\theta\begin{bmatrix}\frac{1}{2}\\ \frac{1}{2}\end{bmatrix}(2u,2\tau) &= \theta\begin{bmatrix}\frac{1}{2}\\ \frac{1}{2}\end{bmatrix}(\tau,2\tau)\times\frac{\sigma(u)\sigma(u+\frac{1}{2})}{\sigma(\frac{\tau}{2})\sigma(\frac{1}{2}+\frac{\tau}{2})},\\ \theta\begin{bmatrix}0\\ \frac{1}{2}\end{bmatrix}(2u,2\tau) &= \theta\begin{bmatrix}0\\ \frac{1}{2}\end{bmatrix}(0,2\tau)\times\frac{\sigma(u-\frac{\tau}{2})\sigma(u+\frac{1}{2}+\frac{\tau}{2})}{\sigma(-\frac{\tau}{2})\sigma(\frac{1}{2}+\frac{\tau}{2})}.\end{aligned}$$

On the other hand, for the R.H.S. of the resulting relation, we obtain

$$\begin{aligned}\text{R.H.S.} &= \frac{\mathrm{Det}\{K^-(u+\eta)\}}{\Delta_2(u+\eta)}tr\left(VK^-(-u-\eta)V\right)\\ &= \frac{\mathrm{Det}\{K^-(u+\eta)\}}{\Delta_2(u+\eta)}tr\left(V^2K^-(-u-\eta)\right)\\ &= -\frac{\mathrm{Det}\{K^-(u+\eta)\}}{\Delta_2(u+\eta)}tr\left(K^-(-u-\eta)\right)\\ &= -\frac{\mathrm{Det}\{K^-(u+\eta)\}}{\Delta_2(u+\eta)}\frac{\sigma(2u+2\eta)}{\sigma(u+\eta)}.\end{aligned} \tag{A.7}$$

Comparing with (A.6) and (A.7), we have

$$\frac{\mathrm{Det}\{K^-(u+\eta)\}}{\Delta_2(u+\eta)}=\frac{\sigma(2u)}{\sigma(\eta)}. \tag{A.8}$$

Now (3.13) follows from (A.2) and (A.8). Similarly one can prove (3.14) using (2.16). Finally, (A.5) and (A.8) give rise to (4.11), and (4.12) can be similarly be proven from (2.16).

Appendix B: Constraint condition (5.16)

One can easily check that both forms (5.15) of eigenvalues of $t(u)$ satisfy the first quasi-periodicity of (5.2) as required. Now we investigate the second quasi-periodic property. The definitions (5.6) and (5.7) of $\{H_i^{(\pm)}(u|\{\epsilon_l^{(\gamma)}\})\}$ imply

$$H_1^{(\pm)}(u+\tau|\{\epsilon_l^{(\gamma)}\})=e^{-2i\pi((N+3)(2u+\tau)+4\eta)}e^{-2i\pi\left(\pm\sum_{\gamma=\pm}\sum_{l=1}^{3}\epsilon_l^{(\gamma)}\alpha_l^{(\gamma)}\right)}H_1^{(\pm)}(u|\{\epsilon_l^{(\gamma)}\}),$$
$$H_2^{(\pm)}(u+\tau|\{\epsilon_l^{(\gamma)}\})=e^{-2i\pi((N+3)(2u+\tau)+(2N+2)\eta)}e^{-2i\pi\left(\mp\sum_{\gamma=\pm}\sum_{l=1}^{3}\epsilon_l^{(\gamma)}\alpha_l^{(\gamma)}\right)}H_2^{(\pm)}(u|\{\epsilon_l^{(\gamma)}\}).$$

Keeping the above quasi-periodic properties and the definition (3.20) of $Q(u)$ in mind, in order that (5.15) have the second property of (5.2) one needs that the boundary parameters $\{\alpha_l^{(\gamma)}\}$ satisfy the following constraint

$$\sum_{\gamma=\pm}\sum_{l=1}^{3}\epsilon_l^{(\gamma)}\alpha_l^{(\gamma)}=k\eta \quad \mathrm{mod}(1), \tag{B.1}$$

where k is an integer such that $|k|\le N-1$ and $N-1+k$ being even. For such integer k, let us introduce two non-negative integers $M^{(\pm)}$: $M^{(\pm)}=\frac{1}{2}(N-1\mp k)$. Moreover, associated respectively with $H_i^{(\pm)}(u|\{\epsilon_l^{(\gamma)}\})$, one introduces $Q^{(\pm)}(u)$,

$$Q^{(\pm)}(u)=\prod_{j=1}^{M^{(\pm)}}\sigma(u-u_j^{(\pm)})\sigma(u+u_j^{(\pm)}+\eta).$$

Hence the eigenvalues of the transfer matrix take the following forms:

$$H_1^{(\pm)}(u|\{\epsilon_l^{(\gamma)}\})\,\frac{Q^{(\pm)}(u+\eta)}{Q^{(\pm)}(u)}+H_2^{(\pm)}(u|\{\epsilon_l^{(\gamma)}\})\,\frac{Q^{(\pm)}(u-\eta)}{Q^{(\pm)}(u)}. \tag{B.2}$$

At this stage, we still have freedom to chose the discrete parameters $\{\epsilon_l^{(\gamma)}\}$. Now we apply the semi-classical property (5.5) of $\Lambda(u)$ to obtain a restriction to this freedom.

For this purpose, let us introduce $\Lambda^{(\pm)}(u)$, corresponding to (B.2),

$$\Lambda^{(\pm)}(u)=H_1^{(\pm)}(u|\{\epsilon_l^{(\gamma)}\})\,\frac{Q^{(\pm)}(u+\eta)}{Q^{(\pm)}(u)}+H_2^{(\pm)}(u|\{\epsilon_l^{(\gamma)}\})\,\frac{Q^{(\pm)}(u-\eta)}{Q^{(\pm)}(u)}, \tag{B.3}$$

and define $\bar{\alpha}_l^{(\gamma)} = \lim_{\eta\to 0}\alpha_l^{(\gamma)}$. Since the value of the discrete parameters $\{\epsilon_l^{(\gamma)}\}$ does not change when taking the limit of $\eta \to 0$, the constraint (B.1) in this limit becomes

$$\sum_{\gamma=\pm}\sum_{l=1}^{3}\epsilon_l^{(\gamma)}\bar{\alpha}_l^{(\gamma)} = 0 \quad \mathrm{mod}(1). \tag{B.4}$$

Substituting (B.3) into the semi-classical property (5.5) of the eigenvalues of the fundamental transfer matrix $t(u)$, we have for the L.H.S. of the resulting relation,

$$\begin{aligned}\text{L.H.S.} &= \lim_{\eta\to 0}\left\{\sigma^{2N}(\eta)\Lambda^{(\pm)}(u)\right\} \\ &= \sigma^{2N}(u)\left\{\prod_{\gamma=\pm}\prod_{l=1}^{3}\frac{\sigma(u\pm\epsilon_l^{(\gamma)}\bar{\alpha}_l^{(\gamma)})}{\sigma(\epsilon_l^{(\gamma)}\bar{\alpha}_l^{(\gamma)})} + \prod_{\gamma=\pm}\prod_{l=1}^{3}\frac{\sigma(u\mp\epsilon_l^{(\gamma)}\bar{\alpha}_l^{(\gamma)})}{\sigma(\epsilon_l^{(\gamma)}\bar{\alpha}_l^{(\gamma)})}\right\}.\end{aligned}$$

Comparing both side of the resulting relation, (5.5) is equivalent to the following relation

$$\prod_{\gamma=\pm}\prod_{l=1}^{3}\frac{\sigma(u\pm\epsilon_l^{(\gamma)}\bar{\alpha}_l^{(\gamma)})}{\sigma(\epsilon_l^{(\gamma)}\bar{\alpha}_l^{(\gamma)})} + \prod_{\gamma=\pm}\prod_{l=1}^{3}\frac{\sigma(u\mp\epsilon_l^{(\gamma)}\bar{\alpha}_l^{(\gamma)})}{\sigma(\epsilon_l^{(\gamma)}\bar{\alpha}_l^{(\gamma)})} = \lim_{\eta\to 0}\left\{tr(K^+(u)K^-(u))\right\}. \tag{B.5}$$

Keeping the constraint (B.4) among $\{\bar{\alpha}_l^{(\gamma)}\}$, after straightforward calculation, we find that (B.5) is satisfied if and only if the following constraint among the discrete parameters $\{\epsilon_l^{(\gamma)}\}$ were fulfilled

$$\prod_{\gamma=\pm}\prod_{l=1}^{3}\epsilon_l^{(\gamma)} = -1. \tag{B.6}$$

(B.1) and (B.6) are nothing but the constraints listed in (5.16).

Appendix C: Trigonometric limit

In this Appendix, we consider the trigonometric limit $\tau \to +i\infty$ of our result. The definition of the elliptic functions (2.1)-(2.2) imply

$$\sigma(u+\frac{\tau}{2}) = e^{-i\pi(u+\frac{1}{2}+\frac{\tau}{4})}\,\theta\left[\begin{array}{c}0\\ \frac{1}{2}\end{array}\right](u,\tau), \tag{C.1}$$

and the following asymptotic behaviors

$$\lim_{\tau\to+i\infty}\sigma(u) = -2e^{\frac{i\pi\tau}{4}}\sin\pi u + \ldots, \tag{C.2}$$

$$\lim_{\tau\to+i\infty}\theta\left[\begin{array}{c}0\\ \frac{1}{2}\end{array}\right](u,\tau) = 1 + \ldots. \tag{C.3}$$

The above asymptotic behaviors lead to the well-known result:

$$\lim_{\tau\to+i\infty} R(u) = \frac{1}{\sin\,\pi\eta}\begin{pmatrix} \sin\pi(u+\eta) & & & \\ & \sin\,\pi u & \sin\,\pi\eta & \\ & \sin\,\pi\eta & \sin\,\pi u & \\ & & & \sin\pi(u+\eta) \end{pmatrix}. \qquad \text{(C.4)}$$

After reparameterizing the boundary parameters

$$\alpha_1^{(\mp)} = \pm\alpha_\mp, \quad \alpha_2^{(\mp)} = \mp\beta_\mp + \frac{1}{2}, \quad \alpha_3^{(\mp)} = -\theta_\mp + \frac{1}{2} + \frac{\tau}{2}, \qquad \text{(C.5)}$$

and using (C.1)-(C.3), one has

$$\lim_{\tau\to+i\infty} K^-(u) \equiv K^-_{(t)}(u) = \frac{1}{2\sin\pi\alpha_-\cos\pi\beta_-}\{2\sin\pi\alpha_-\cos\pi\beta_-\cos\pi u\, I + 2i\cos\pi\alpha_-\sin\pi\beta_-\sin\pi u\,\sigma^z + \sin 2\pi u\,(\cos\pi\theta_-\,\sigma^x - \sin\pi\theta_-\,\sigma^y)\}, \qquad \text{(C.6)}$$

$$\lim_{\tau\to+i\infty} K^+(u) \equiv K^+_{(t)}(u) = K^-_{(t)}(-u-\eta)\Big|_{(\alpha_-,\beta_-,\theta_-)\to(-\alpha_+,-\beta_+,\theta_+)}. \qquad \text{(C.7)}$$

Hence our R-matrix and K-matrices, when taking the trigonometric limit, reduce to the corresponding trigonometric ones used in [5] after a rescaling of the corresponding parameters. In order for the constraint (5.16) to be still satisfied after the limit, one needs further to require that $\epsilon_3^{(-)} = -\epsilon_3^{(+)}$. Then, the resulting constraint becomes that in [5]. Moreover, our $\{H_i^{(\pm)}(u|\{\epsilon_l^{(\gamma)}\})\}$ in the limit give rise to the corresponding trigonometric ones in [5] up to some constants (due to the constant factors appearing in (C.4), (C.6)-(C.7)). Therefore, our result recovers that of [5] in the trigonometric limit.

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